## 論文内容の要旨

論文題目 Interface Optimization for Organic Electronic Devices by Self-assembled Monolayers and Conductive Polymers

[ 自己集合単分子膜および導電性ポリマーによる有機エレクトロニクスデバイスの界面最適化に関する研究]

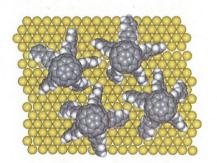
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This thesis describes a comprehensive investigation of the interface optimization of organic electronic devices by self-assembled monolayers and conductive polymers.

In Chapter 2 the novel characterization technique of photoelectron yield spectroscopy (PYS) was calibrated for work function determination. The work function is one of the most important electronic properties of inorganic substrates used in organic electronic devices. This chapter proves that the PYS technique is extremely useful and reliable in the rapid determination of work functions on a variety of substrates.

Chapter 3 describes new fullerene self-assembled monolayers (SAMs) for

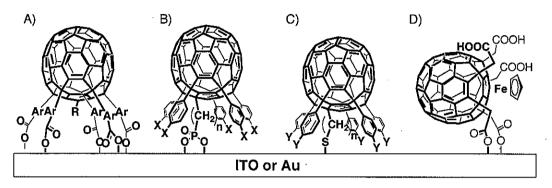
functionalization of gold substrates. The generation of clean fullerene SAMs has been very challenging so far because of facile cluster and multilayer formation. This issue was solved in this chapter by a special fullerene design with an arene cone spacer and alkyl thiol linker leading to clean SAM formation. The optoelectronic properties of these SAMs were investigated, which allowed further insights in the SAM-forming process and confirmed the structure as displayed in Figure 1.



**Figure 1.** Top view of fullerene SAM on gold.

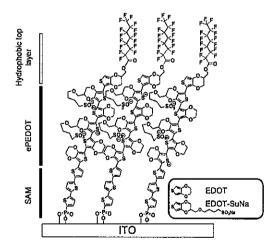
In Chapter 4 the influences of SAMs on surface properties and work function of inorganic substrates were investigated in great detail. Although being of high importance, a quantitative study of SAMs of chemically bound compounds has been difficult so far. This problem was solved by the use of rationally designed "umbrella" fullerene compounds that were self-assembled on indium-tin oxide (ITO) and gold

(Scheme 1). Molecular and supramolecular influences on the work function and water contact angles were studied by variation of specific parameters such as ionization potential, molecular length or surface coverage. This made it possible to confirm the theories commonly used for describing work function shifts and correlate them to the molecular level reality.



Scheme 1. A)-C) Three classes of model compounds for SAMs standing upright on ITO and gold. D) Compound with different orientation on ITO (Ar =  $-C_6H_4$ -,  $-C_6H_4$ - $-C_6H_4$ -; R = Me, FeC<sub>5</sub>H<sub>5</sub>; n = 3, 4, 6; X = H, Ph, NMe<sub>2</sub>, CF<sub>3</sub>; Y = H, Ph).

In Chapter 5 the influences of work function and other surface properties such as hydrophobicity surface on the device performance of organic electronic devices organic photovoltaics, OPVs) is described. Current anode buffer layers have disadvantages that need to be overcome to reach high device efficiencies. For that purpose a novel and highly conductive polyelectrolyte with a tunable work function (4.4-5.2 eV), tunable hydrophobicity, high conductivity, transparency and low surface roughness is introduced. detailed



**Figure 2.** Optimized layered anode buffer layer with tunable work function and surface energy.

investigation of this novel polymer and its influence on OPV performance was performed. The layered architecture of this novel polymer was made possible by electropolymerization (Figure 2) and is believed to be useful for future applications in organic electronic devices with the need for specifically optimized parameters.